

Thermal Entanglement of a Spin-1/2 Ising-Heisenberg Model on a Symmetrical Diamond Chain

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Abstract. The entanglement quantum properties of a spin-1/2 Ising-Heisenberg model on a symmetrical diamond chain were analyzed. Due to the separable nature of the Ising-type exchange interactions between neighboring Heisenberg dimers, calculation of the entanglement can be performed exactly for each individual dimer. Pairwise thermal entanglement was studied in terms of the isotropic Ising-Heisenberg model, and analytical expressions for the concurrence (as a measure of bipartite entanglement) were obtained. The effects of external magnetic field H and next-nearest neighbor interaction J_m between nodal Ising sites were considered. The ground-state structure and entanglement properties of the system were studied in a wide range of the coupling constant values. Various regimes with different values of the ground-state entanglement were revealed, depending on the relation between competing interaction strengths. Finally, some novel effects, such as the two-peak behavior of concurrence versus temperature and coexistence of phases with different values of magnetic entanglement were observed.

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1. Introduction

During the last two decades low-dimensional magnetic materials with competing interactions or geometrical frustration have become an intriguing research object. Particularly, these materials exhibit a rich variety of unusual ground states and thermal properties, as a result of zero and finite temperature phase transitions [1–5]. As attractive models among these systems, one should mention the ones, having a diamond-chain structure. The latter consists of diamond-shaped topological units along the chain (Fig. 1). It has been observed that the compounds $A_3Cu_3(PO_4)_4$ with $A=Ca, Sr$ [6], $Bi_4Cu_3V_2O_{14}$ [7] and $Cu_3(TeO_3)_2Br_2$ [8] can be nicely modeled by the Heisenberg diamond chain. Besides, recent experimental results on the natural mineral azurite ($Cu_3(CO_3)_2(OH)_2$) [9] showed that Cu^{2+} ions of this material form a spin-1/2 diamond chain. Furthermore, the discovery of a plateau at 1/3 of the saturation value in the low-temperature magnetization curve [9, 10] has triggered an intensive interest in the magnetic properties of azurite [11, 12]. Azurite falls into the class of geometrically frustrated magnets. However, the question of the strength and the type of exchange interactions for this natural mineral, despite the long-standing interest, is still open. The first diamond spin chain was explored under a symmetrical condition $J_1 = J_3$ [13] that predicted magnetization plateaus both at 1/3 and 1/6 of saturation [14]. The frustrated diamond chain with ferromagnetic interactions $J_1, J_3 < 0$ and antiferromagnetic interaction $J_2 > 0$ was also investigated theoretically [15]. Other exchange interactions, like an additional cyclic four-spin [16] and J_m interaction between monomeric units (the so called generalized diamond chain) [17] were considered. Additionally, the importance of an anisotropic exchange and Dzyaloshinskii-Moriya interaction [18] or interchain coupling [19] was discussed. To sum up, note that the theory predictions for certain values of exchange coupling constants within a relatively broad range can fit the experimental results. The controversy on these values seems to be cleared up only recently (the latest comparison of experimental and theoretical results can be found in Ref. [20]).

Motivated by the controversies discussed above and the fact that different compounds can be described by means of a diamond chain, we shall explore systematically the generalized symmetrical spin-1/2 diamond chain with various competing interactions in a magnetic field. Unfortunately, the rigorous theoretical treatment of geometrically frustrated quantum Heisenberg models is difficult to fulfil. The problem arises due to a non-commutability of spin operators involved in the Heisenberg Hamiltonian. This is also a primary cause of a presence of quantum fluctuations. Owing to this fact, we will use the recently proposed geometrically frustrated Ising-Heisenberg diamond chain model [21–23]. The latter suggests to overcome the mathematical difficulties by introducing the Ising spins at the nodal sites and the Heisenberg dimers on the interstitial decorating sites of the diamond chain (Fig. 1). For understanding of the properties of underlying purely quantum models it is required to obtain an analytic expression for all thermodynamic functions of the model. Note that some exactly solvable models with Ising and Heisenberg bonds can also provide satisfactory quantitative picture [24].

In the present paper we shall mainly deal with the quantum entanglement properties of the spin-1/2 Ising-Heisenberg model on a generalized symmetrical diamond chain. It is well-known, that the entanglement is a generic feature of quantum correlations in systems, that cannot be quantified classically [25, 26]. It provides a new perspective for understanding the quantum phase transitions (QPTs)

and collective phenomena in many-body and condensed matter physics. This problem, which has been under scrutiny for nearly two decades, has recently attracted much attention [27–31]. A new line research points to a relation between the entanglement of a many-particle system and the existence of the QPTs and scaling [32, 33]. On the other hand, the study of entanglement in solid state physics is of a great relevance to the area of Quantum Information and Quantum Computation, since many proposals of quantum chips are solid state-based. Although it was believed that the entanglement should not manifest itself in macroscopic objects (because of a large number of constituents interacting with the surroundings that induce the decoherence phenomena), it was theoretically demonstrated that entangled states can exist in solids at finite temperatures. This kind of entanglement is referred to in literature as "the thermal entanglement" [27]. And afterwards a few experimental evidences have been reported for low-dimensional spin systems [34], confirming the presence of entanglement in solid state materials.

Returning to the spin-1/2 Ising-Heisenberg model on a diamond chain we remark that the nodal Ising spins represent a barrier for quantum fluctuations. On the other hand, taking into account that each Heisenberg dimer interacts with its neighboring dimer through the Ising-type, i.e. classical exchange interaction, we find that the states of two adjacent dimers become separable (disentangled) [25]. Thus, we can calculate the concurrence (the measure of pairwise entanglement [35]), which characterizes quantum features of the system, for each dimer separately. The main objective of the paper is to reveal different regimes of the symmetrical diamond chain and to analyze new quantum effects (such as double peak behavior in the concurrence versus temperature curves, existence of magnetic entanglement [27] of two different values).

The rest of the paper is organized as follows: we start in Sec. 2 by obtaining concurrence as a measure of entanglement of the spin-1/2 Ising-Heisenberg model on a generalized symmetrical diamond chain. The ground-state structure and the entanglement features of the ideal diamond chain ($J_1 = J_3$, $J_m = 0$) are discussed in Sec. 2.1. The following section contains similar results with the incorporation of J_m interaction. Some comments and concluding remarks are given in Sec. 4.

2. Concurrence and thermal entanglement of the spin-1/2 Ising-Heisenberg model on a generalized symmetrical diamond

We consider the spin- $\frac{1}{2}$ Ising-Heisenberg model on a generalized symmetrical diamond chain ($J_1 = J_3 = J$), which consists of monomeric and dimeric sites (empty and full circles in Fig. 1, respectively). Within the proposed Ising-Heisenberg model, the monomeric (nodal) sites are occupied by Ising spins, while the dimeric sites by Heisenberg-type spins. The Hamiltonian can be written as follows:

$$\mathcal{H} = \sum_{k=1}^N \mathcal{H}_k = \sum_{k=1}^N \left[J_2 \mathbf{S}_{k_1} \mathbf{S}_{k_2} + J(\mu_k^z + \mu_{k+1}^z)(S_{k_1}^z + S_{k_2}^z) + J_m \mu_k^z \mu_{k+1}^z - H \left(S_{k_1}^z + S_{k_2}^z + \frac{\mu_k^z + \mu_{k+1}^z}{2} \right) \right], \quad (1)$$

where the summations run over clusters (Fig. 1), \mathcal{H}_k represents the Hamiltonian of the k -th cluster, $\mathbf{S}_k = (S_k^x, S_k^y, S_k^z)$ denotes the Heisenberg spin- $\frac{1}{2}$ operator, μ_k is the Ising spin. Considering, that each Ising spin belongs simultaneously to two

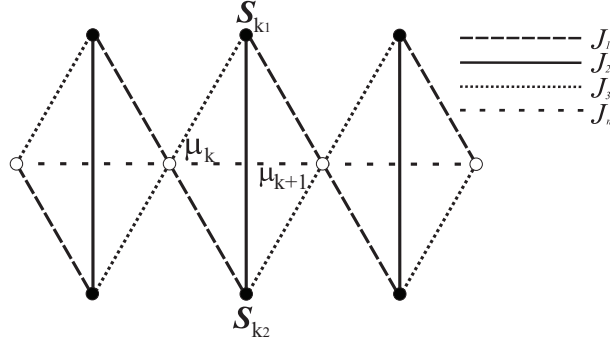


Figure 1. A cross-section of a generalized symmetrical diamond chain (k labels the number of the cluster). The empty (monomeric units) and full circles (dimeric units) denote lattice positions of the Heisenberg and Ising spins (within the proposed Ising-Heisenberg model), respectively. Solid lines schematically reproduce the Heisenberg J_2 interactions between dimeric units, while the broken ones label the Ising-type (nearest-neighbor J_1 , J_3 and next-nearest neighbor J_m) interactions.

clusters, we have taken a $1/2$ factor for the Ising spins in the last term of (1), which incorporates the effects of external magnetic field. $J, J_2, J_m > 0$ corresponds to the antiferromagnetic couplings. The system will be strongly frustrated due to the chain's geometry and existence of competing interactions J, J_2 and J_m . When $J_m = 0$ we deal with the so called ideal diamond chain [21]. Before introducing the calculations and discussion we would like to emphasize the fact which was already discussed in Sec. 1: the states of two neighboring Heisenberg dimers (with interaction J_2) are separable (disentangled), because of a classical character of the coupling between them (by means of the Ising spin). Hence we can calculate the entanglement for each of the dimers individually. Note, that a different approach of a mean-field-like treatment, based on the Gibbs-Bogoliubov inequality was used in Ref. [36], where all the couplings between the diamond chain sites were chosen to be of a quantum (Heisenberg-type) character.

Here we use concurrence (as a measure of bipartite entanglement [35]) of the Heisenberg dimers by tracing out the Ising spins in each cluster. For the construction of eigenvectors of each cluster we will take into account that \mathcal{H}_k possesses a symmetry corresponding to the permutations $\mu_k \leftrightarrow \mu_{k+1}$ and $\{\mu_k \leftrightarrow \mu_{k+1}; \mathbf{S}_{k1} \leftrightarrow \mathbf{S}_{k2}\}$. Besides, the Hilbert space of the cluster $\mathcal{H}_{cluster}$ can be presented as $\mathcal{H}_{cluster} = \mathcal{H}_k \otimes \mathcal{H}_{dimer} \otimes \mathcal{H}_{k+1}$, where \mathcal{H}_{k1} , \mathcal{H}_{dimer} , \mathcal{H}_{k2} denotes the Hilbert spaces of μ_k , Heisenberg dimer and μ_{k+1} respectively. We obtain the following eigenvectors, due to the symmetries and Hilbert space structure (hereafter, the letter k labels the number of the cluster):

$$\begin{aligned} |\psi_1\rangle &= \frac{1}{\sqrt{2}}(|\uparrow_{k1} \otimes \downarrow_{k2}\rangle + |\downarrow_{k1} \otimes \uparrow_{k2}\rangle) \otimes |\uparrow_k \uparrow_{k+1}\rangle; \\ |\psi_2\rangle &= \frac{1}{\sqrt{2}}(|\uparrow_{k1} \otimes \downarrow_{k2}\rangle + |\downarrow_{k1} \otimes \uparrow_{k2}\rangle) \otimes (|\uparrow_k \downarrow_{k+1}\rangle + |\downarrow_k \uparrow_{k+1}\rangle); \\ |\psi_3\rangle &= \frac{1}{\sqrt{2}}(|\uparrow_{k1} \otimes \downarrow_{k2}\rangle + |\downarrow_{k1} \otimes \uparrow_{k2}\rangle) \otimes (|\uparrow_k \downarrow_{k+1}\rangle - |\downarrow_k \uparrow_{k+1}\rangle); \end{aligned}$$

$$\begin{aligned}
 |\psi_4\rangle &= \frac{1}{\sqrt{2}}(|\uparrow_{k_1} \otimes \downarrow_{k_2}\rangle + |\downarrow_{k_1} \otimes \uparrow_{k_2}\rangle) \otimes |\downarrow_k \downarrow_{k+1}\rangle; \\
 |\psi_5\rangle &= \frac{1}{\sqrt{2}}(|\uparrow_{k_1} \otimes \downarrow_{k_2}\rangle - |\downarrow_{k_1} \otimes \uparrow_{k_2}\rangle) \otimes |\uparrow_k \uparrow_{k+1}\rangle; \\
 |\psi_6\rangle &= \frac{1}{\sqrt{2}}(|\uparrow_{k_1} \otimes \downarrow_{k_2}\rangle - |\downarrow_{k_1} \otimes \uparrow_{k_2}\rangle) \otimes (|\uparrow_k \downarrow_{k+1}\rangle + |\downarrow_k \uparrow_{k+1}\rangle); \\
 |\psi_7\rangle &= \frac{1}{\sqrt{2}}(|\uparrow_{k_1} \otimes \downarrow_{k_2}\rangle - |\downarrow_{k_1} \otimes \uparrow_{k_2}\rangle) \otimes (|\uparrow_k \downarrow_{k+1}\rangle - |\downarrow_k \uparrow_{k+1}\rangle); \\
 |\psi_8\rangle &= \frac{1}{\sqrt{2}}(|\uparrow_{k_1} \otimes \downarrow_{k_2}\rangle - |\downarrow_{k_1} \otimes \uparrow_{k_2}\rangle) \otimes |\downarrow_k \downarrow_{k+1}\rangle; \\
 |\psi_9\rangle &= |\uparrow_{k_1} \otimes \uparrow_{k_2}\rangle \otimes |\uparrow_k \uparrow_{k+1}\rangle; \\
 |\psi_{10}\rangle &= \frac{1}{\sqrt{2}}|\uparrow_{k_1} \otimes \uparrow_{k_2}\rangle \otimes (|\uparrow_k \downarrow_{k+1}\rangle + |\downarrow_k \uparrow_{k+1}\rangle); \\
 |\psi_{11}\rangle &= \frac{1}{\sqrt{2}}|\uparrow_{k_1} \otimes \uparrow_{k_2}\rangle \otimes (|\uparrow_k \downarrow_{k+1}\rangle - |\downarrow_k \uparrow_{k+1}\rangle); \\
 |\psi_{12}\rangle &= |\uparrow_{k_1} \otimes \uparrow_{k_2}\rangle \otimes |\downarrow_k \downarrow_{k+1}\rangle; \\
 |\psi_{13}\rangle &= |\downarrow_{k_1} \otimes \downarrow_{k_2}\rangle \otimes |\uparrow_k \uparrow_{k+1}\rangle; \\
 |\psi_{14}\rangle &= \frac{1}{\sqrt{2}}|\downarrow_{k_1} \otimes \downarrow_{k_2}\rangle \otimes (|\uparrow_k \downarrow_{k+1}\rangle + |\downarrow_k \uparrow_{k+1}\rangle); \\
 |\psi_{15}\rangle &= \frac{1}{\sqrt{2}}|\downarrow_{k_1} \otimes \downarrow_{k_2}\rangle \otimes (|\uparrow_k \downarrow_{k+1}\rangle - |\downarrow_k \uparrow_{k+1}\rangle); \\
 |\psi_{16}\rangle &= |\downarrow_{k_1} \otimes \downarrow_{k_2}\rangle \otimes |\downarrow_k \downarrow_{k+1}\rangle;
 \end{aligned} \tag{2}$$

and the corresponding eigenvalues:

$$\begin{aligned}
 E_1 &= \frac{1}{4}(-2H + J_m + J_2); \quad E_2 = E_3 = -\frac{J_m - J_2}{4}; \\
 E_4 &= \frac{1}{4}(J_m + J_2 + 2H); \quad E_5 = \frac{1}{4}(-2H + J_m - 3J_2); \\
 E_6 &= E_7 = -\frac{J_m + 3J_2}{4}; \quad E_8 = \frac{1}{4}(2H + J_m - 3J_2); \\
 E_9 &= -\frac{3H}{2} + \frac{J_m + J_2}{4} + J; \quad E_{10} = E_{11} = -H - \frac{J_m - J_2}{4}; \\
 E_{12} &= -\frac{H}{2} + \frac{1}{4}(J_m + J_2 - 4J); \quad E_{13} = \frac{H}{2} + \frac{1}{4}(J_m + J_2 - 4J); \\
 E_{14} &= E_{15} = \frac{1}{4}(-J_m + J_2 + 4H); \quad E_{16} = \frac{3H}{2} + \frac{J_m + J_2}{4} + J.
 \end{aligned} \tag{3}$$

We study *concurrence* $C(\rho)$, to quantify pairwise entanglement [35], defined as

$$C(\rho) = \max\{\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0\}, \tag{4}$$

where λ_i 's are the square roots of the eigenvalues of the corresponding operator for the density matrix

$$\tilde{\rho} = \rho_{12}(\sigma_1^y \otimes \sigma_2^y) \rho_{12}^*(\sigma_1^y \otimes \sigma_2^y) \tag{5}$$

in descending order. Since we consider pairwise entanglement, we should use the reduced density matrix ρ_{12} , by tracing out two (of four) spins of the cluster. The

reduced density matrix ρ_{12} is defined as [37]

$$\rho_{12} = \sum_{\alpha} \langle \alpha | \rho | \alpha \rangle. \quad (6)$$

In this equation $|\alpha\rangle$ denotes basis vectors of the Hilbert space associated with the system, with respect to which the density matrix is reduced. The summation runs over all these basis vectors. Since in our case we make reduction with respect to two spins, $|\alpha\rangle = \{|\downarrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\uparrow\uparrow\rangle\}$.

It is obvious that the only entangled pair is formed by the Heisenberg spins. Other pairs are disentangled (separable) because of the classical (diagonal) character of the Ising-type interaction between them. Hence we will be interested in the reduced density matrix, constructed by tracing out two Ising-type spins μ_k and μ_{k+1} . In other words, $\rho_{k_{12}} = \text{Tr}_{\{\mu_k, \mu_{k+1}\}} \rho_k$ and the full density matrix ρ_k of the k -th cluster is defined as (here and further Boltzmann constant is set to be $k_B = 1$)

$$\rho_k = \frac{1}{Z_k} \sum_{i=1}^{16} \exp(-E_i/T) |\psi_i\rangle \langle \psi_i|, \quad (7)$$

where Z_k is the partition function:

$$\begin{aligned} Z_k = \text{Tr} \rho_k = e^{-\frac{6H+J_m+4J+J_2}{4T}} & \left(2e^{\frac{H+J_m+2J}{2T}} + 2e^{\frac{3H+J_m+2J}{2T}} + \right. \\ & 2e^{\frac{5H+J_m+2J}{2T}} + 2e^{\frac{3H+J_m+2J+2J_2}{2T}} + e^{\frac{H+J}{T}} + e^{\frac{2(H+J)}{T}} + \\ & \left. e^{\frac{2H+J}{T}} + e^{\frac{H+2J}{T}} + e^{\frac{H+J+J_2}{T}} + e^{\frac{2H+J+J_2}{T}} + e^{\frac{3H}{T}} + 1 \right). \end{aligned} \quad (8)$$

Using the definition (6), the basis vectors $|\alpha\rangle = \{|\downarrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\uparrow\uparrow\rangle\}$ we construct the reduced density matrix $\rho_{k_{12}}$ of the k -th cluster:

$$\rho_{k_{12}} = \begin{pmatrix} u & 0 & 0 & 0 \\ 0 & w & y & 0 \\ 0 & y^* & w & 0 \\ 0 & 0 & 0 & v \end{pmatrix}, \quad (9)$$

where

$$\begin{aligned} u &= 2e^{\frac{4H+J_m-J_2}{4T}} + e^{-\frac{2H+J_m-4J+J_2}{4T}} + e^{-\frac{6H+J_m+4J+J_2}{4T}}, \\ v &= e^{-\frac{6H+J_m+4J+J_2}{4T}} \left(2e^{\frac{H+J_m+2J}{2T}} + e^{\frac{H+2J}{T}} + 1 \right), \\ w &= \frac{1}{2} \left(e^{\frac{J_2}{T}} + 1 \right) e^{-\frac{2H+J_m+J_2}{4T}} \left(2e^{\frac{H+J_m}{2T}} + e^{H/T} + 1 \right), \\ y &= -\frac{1}{2} \left(e^{\frac{J_2}{T}} - 1 \right) e^{-\frac{2H+J_m+J_2}{4T}} \left(2e^{\frac{H+J_m}{2T}} + e^{H/T} + 1 \right). \end{aligned} \quad (10)$$

The density matrix $\rho_{k_{12}}$ in Eq. (9) has a form of a so called X -state [38], since the Hamiltonian \mathcal{H}_k is translationary invariant with a symmetry $[S_z, \mathcal{H}_k] = 0$ ($S_z = 1/2(\mu_k^z + \mu_{k+1}^z) + S_{k_1}^z + S_{k_2}^z$) [39]. The concurrence $C(\rho)$ of such an X -state density matrix has the following form [40]:

$$C(\rho) = \frac{2}{Z} \max(|y| - \sqrt{uv}, 0). \quad (11)$$

We note here that the reduced density matrix $\rho_{k_{12}}$ of any pair of spins, different from the Heisenberg dimer has no non-diagonal elements, responsible for the quantum

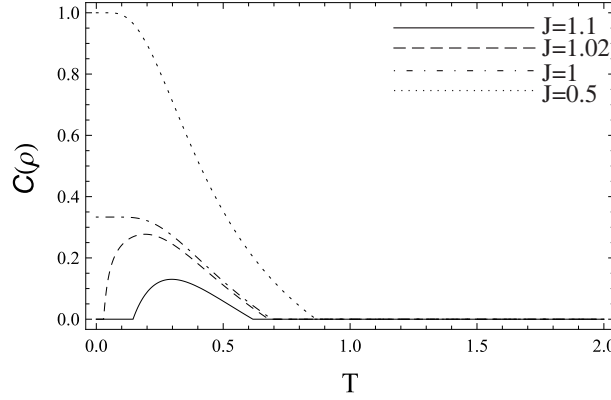


Figure 2. Concurrence $C(\rho)$ versus temperature T for $J_2 = 1$, $J_m = 0$, $H = 0$, and different values of J .

correlations, i.e. entanglement (see (11)). Thus we conclude, that there is no entanglement between a pair of spins which contains at least one Ising spin.

In Eq. (3), one finds a set of states with maximum value of entanglement, for which the Heisenberg dimer is in a singlet or a triplet state (ψ_i 's with $i = 1, \dots, 8$). As for the rest of the states (ψ_i 's with $i = 9, \dots, 16$) the Heisenberg dimer is in a separable state and therefore these ψ_i 's are non-entangled ones.

2.1. Ideal diamond chain

In this section we proceed to the investigation of entanglement features of a dimeric unit of an ideal diamond chain ($J_m = 0$). First, we study the behavior of $C(\rho)$ at $H = 0$. We will discuss here three regimes, depending on the value of $J - J_2$: $J - J_2 > 0$, $J - J_2 < 0$ and $J - J_2 = 0$. In the first case, as one finds out from (3), the ground state contains two-fold degenerate states ψ_{12} and ψ_{13} . Since these states are factorable, the corresponding dependency curve of $C(\rho)$ from temperature T starts from $C(\rho) = 0$ (Fig. 2). Furthermore, the entanglement can be invoked by increasing the temperature (for values of $J - J_2$ close to 0). This happens since the contribution of entangled states in the mixture ρ_k increases with the growth of temperature T . The local maximum, appearing here arises due to the optimal thermal mixing of all eigenstates in the system. This maximum becomes narrower and smaller and gradually vanishes by increasing $J - J_2$. But the value of $J - J_2$ corresponding to disappearing of $C(\rho)$ also depends on the value of J_2 (e.g. for $J_2 = 1$, $J - J_2 \approx 0.2$). The latter becomes obvious, if one takes into account that J_2 , being the coupling constant of the Heisenberg type interaction between dimeric units, is responsible for the strength of quantum correlations between Heisenberg spins. We would like to emphasize here that in the case $J - J_2 > 0$ the system exhibits weak ($0 < J_2 < J$) or no frustration ($J_2 < 0$).

In the second case, when $J - J_2 < 0$, the system will obviously manifest more of its quantum nature. Firstly, the dependency curve of $C(\rho)$ from temperature starts from $C(\rho) = 1$ at $T = 0$ (Fig. 2). This happens due to the fact that at zero temperature the maximum entangled states ψ_5 , ψ_6 , ψ_7 and ψ_8 form four-fold degenerate ground state with the value of $C(\rho) = 1$ for the corresponding reduced density matrix $\rho_{k_{12}}$. When

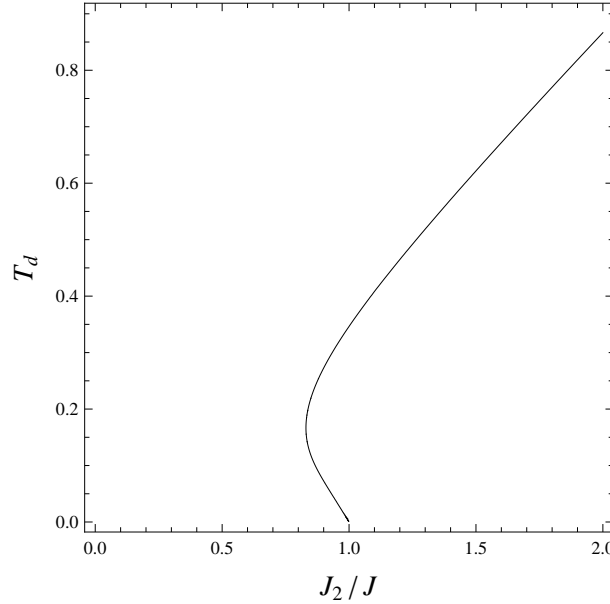


Figure 3. Sudden-death temperature T_d corresponding to the vanishing or arising of entanglement at zero magnetic H versus ratio parameter J_2/J ($J = 0.5$).

the temperature is increased, the concurrence gradually disappears because of the thermal mixing with other states of the system (including the factorable ones). The sudden-death temperature T_d , corresponding to the dying out of quantum correlations in the system can be found through the equation $C(\rho) = 0$. It has the following form:

$$x^{-J} (x^J + 1)^2 = 2 |x^{J_2} - 1|, \quad (12)$$

where $x = e^{1/T}$. The solution can be presented in the form $T_d = J/\log a$ (when $J - J_2 < 0$), where a depends on the ratio parameter J_2/J . Increasing this ratio, a decreases, but the linear dependence on J remains (e.g. when $J_2/J = 2$, $a = \frac{1}{4}(3 + \sqrt{17})$).

Finally, the case $J - J_2 = 0$ can be regarded as a boundary case in the following sense. Here the ground state is six-fold degenerate, containing additionally ψ_{12} and ψ_{13} , besides ψ_5 , ψ_6 , ψ_7 and ψ_8 (in other words all the states as in previous two cases). Since the ψ_{12} and ψ_{13} are factorable, this leads to lower entanglement of the ground state's reduced matrix, that is $C(\rho) = 1/3$ (Fig. 2). Moreover, the above discussed sudden-death temperature T_d is lower, than in the case $J - J_2 < 0$ (although again $T_d = J/\log a$ with $a = 2 + \sqrt{5}$).

On the other hand, as it can be seen from Fig. 2, there are two sudden-death temperatures in the case $J - J_2 > 0$ (corresponding to arising and vanishing of entanglement) [41]. The dependence of T_d on the ratio parameter J_2/J is shown in Fig. 3. In the area $0 < J_2/J < 1$, there are two sudden-death temperatures (as mentioned above), while for the values $J_2/J \geq 1$, the dependence is a linear one.

Our further investigation concerns the effects of the magnetic field H .

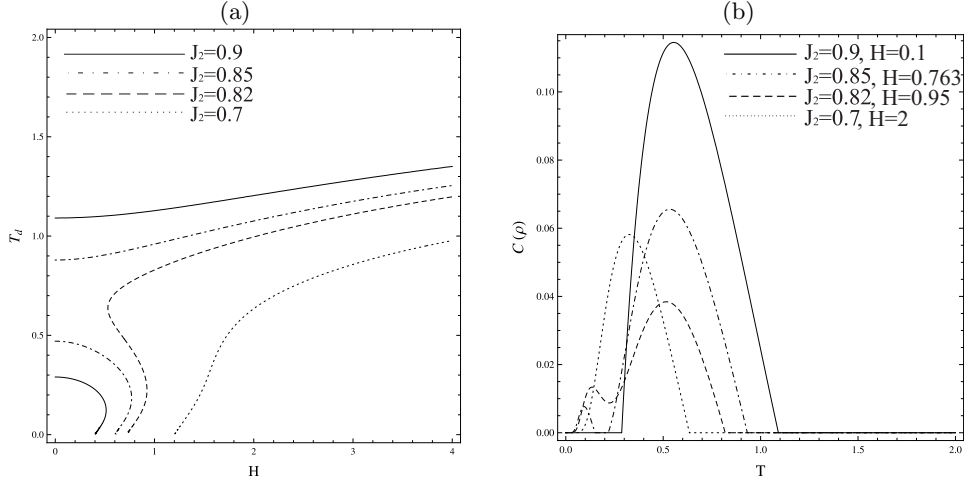


Figure 4. (a) Sudden-death temperature T_d corresponding to the vanishing or arising of entanglement versus magnetic field H for $J = 2$ and different values of J_2 ; (b) Concurrence $C(\rho)$ versus temperature T for $J = 2$ and different values of J_2 and magnetic field H .

Firstly we will discuss how magnetic field affects the above introduced sudden-death temperature T_d . While increasing H , T_d increases too, but it always remains lower than $J_2/\log 3$ (in other words $\lim_{H \rightarrow \infty} T_d = J_2/\log 3$). Another interesting fact is that magnetic field gives a rise to more than two sudden-death temperatures in the case $J - J_2 > 0$ [Fig. 4 (a)] and on the dependence of $C(\rho)$ from temperature T one finds two peaks separated by an area of a zero entanglement [Fig. 4 (b)]. With increasing H the smaller of aforementioned peaks tears apart from $C(\rho) = 0$, starts merging with the bigger one and eventually disappears. An effect of this kind has not been reported yet, to the best of our knowledge. Although a similar two-peak behavior of concurrence was found in dissipative the Lipkin-Meshkov-Glick model versus *magnetic field* [42]. However, when $T \rightarrow 0$, $C(\rho)$ remains finite and becomes zero only at absolute zero temperature $T = 0$ [i.e. there can be not more than three sudden-death temperatures corresponding to disappearing or arising of thermal entanglement, as it can be also seen from Fig. 4 (a)]. In other words in the area of low temperatures the behavior of concurrence is smooth, in contrast with the case when magnetic field is absent.

Now, we concentrate on the dependence of $C(\rho)$ on magnetic field. Because of the above introduced ground state structure, the dependency curve of $C(\rho)$ from magnetic field at zero temperature has a dip at $H = 0$ with $C(\rho) = 1/3$ for $J - J_2 = 0$. There is no dip if $J - J_2 < 0$ (Fig. 5). When Ising-type interaction is stronger than the Heisenberg one ($J - J_2 > 0$), one does not find a magnetic entanglement. Furthermore, magnetic entanglement is of a higher value than that at zero magnetic field in the case $J - J_2 = 0$. This happens due to the fact that ground state here is two-fold degenerated and contains ψ_5 and ψ_{12} with the value $C(\rho) = 1/2$ for the corresponding reduced density matrix. $C(\rho)$ becomes zero for the case $J - J_2 \leq 0$ at the values of H , corresponding to saturation field, that is when the non-entangled state $\uparrow\uparrow\uparrow\uparrow$ (in the area $H > 0$) or $\downarrow\downarrow\downarrow\downarrow$ (in the area $H < 0$) becomes the ground state. One can find the described values of H from the conditions $E_9 = E_5$ and $E_{16} = E_8$, giving $H_s^+ = J + J_2$

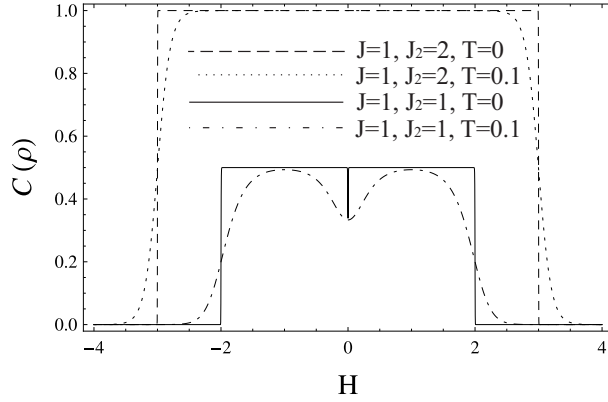


Figure 5. Concurrence $C(\rho)$ versus magnetic field H for different values of temperature, J_2 and J .

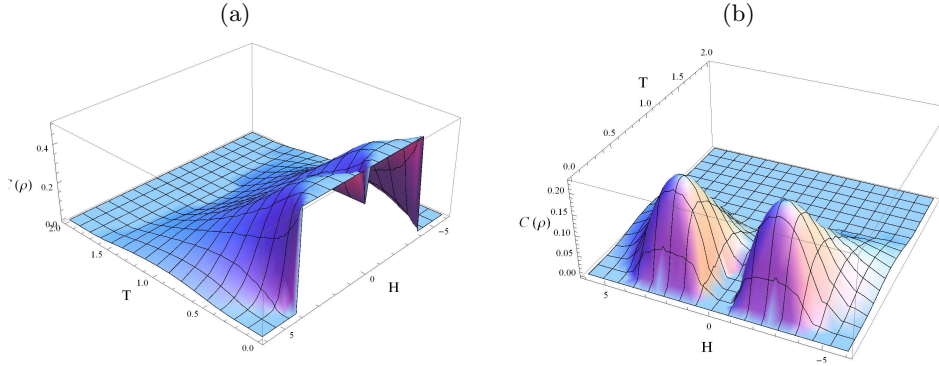


Figure 6. Concurrence $C(\rho)$ versus magnetic field H and temperature T for (a) $J_2 = 2$ and $J = 2$; (b) $J_2 = 1.7$ and $J_1 = J_3 \equiv J = 2$.

and $H_s^- = -J - J_2$, respectively. Thermal effects smooths the step-like behavior of concurrence in the case when $J - J_2 \geq 0$ and induces thermal entanglement when $J - J_2 > 0$ (see Fig. 2). The further increase of temperature causes the quantum correlations eventually dying out for the both cases.

Summarizing, in Fig. 6 we also plot three-dimensional dependencies of the concurrence $C(\rho)$ versus temperature T and magnetic field H .

3. Incorporation of J_m interaction

In this section we will study the effects of the next-nearest neighbor interaction J_m between the Ising spins of the cluster, using the full expression for (10) and (11). We will start with the discussion of the ground state structure for the case $H = 0$ and $J - J_2 > 0$. It turns out that here one can distinguish two regimes. First, when $0 < J_m < 2(J - J_2)$, frustrated ground state contains two-fold degenerate ψ_{12} and ψ_{13} and thus the dependency curve of $C(\rho)$ from temperature starts up at $C(\rho) = 0$. However, the thermal effects can cause the thermal entanglement for the values

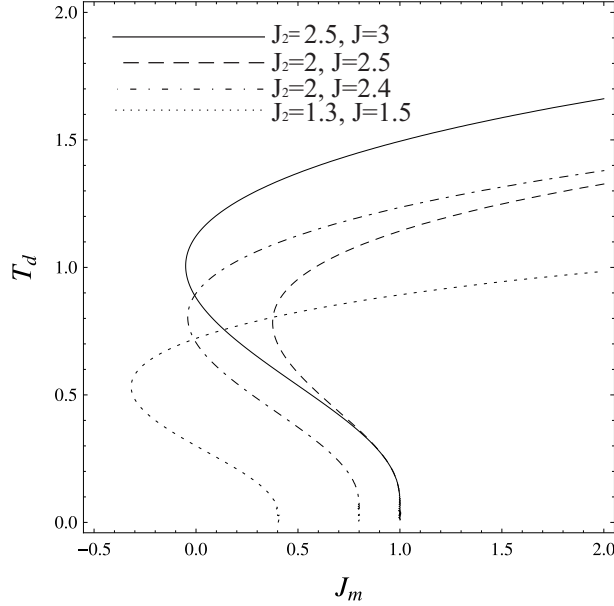


Figure 7. Sudden-death temperature T_d corresponding to the vanishing or arising of entanglement versus J_m for $H = 0$ and different values of J_2 and $J = 2$.

of J_m , close to $2(J - J_2)$ (but remaining $J_m < 2(J - J_2)$). One finds two sudden-death temperatures on the dependency curve of $C(\rho)$ from T (Fig. 7). This effect can be understood from the following discussion. The ground state consists of four-fold degenerate states ψ_6 , ψ_7 , ψ_{12} and ψ_{13} , for the case $J_m = 2(J - J_2)$. Although this mixture contains maximum entangled states ψ_6 and ψ_7 , the corresponding density matrix for this ground state gives $C(\rho) = 0$. By increasing temperature, one obtains the thermal mixing of states which leads to a higher contribution of entangled states. This contribution, however, becomes less, when the values of J_m are considerably higher than $2(J - J_2)$. Thus, with increasing the difference of J_m and $2(J - J_2)$, the local maximum becomes narrower and eventually disappears.

In the opposite case, when $J_m > 2(J - J_2)$, the frustrated ground state is two-fold degenerate, but with ψ_6 and ψ_7 , hence above mentioned curve of $C(\rho)$ starts from $C(\rho) = 1$. We find only one sudden-death temperature here, which increases with the growth of J_m (Fig. 7). In other words, the qualitative picture remains the same as for the case $J_m = 0$.

$C(\rho)$ is of a maximum value ($C(\rho) = 1$) at zero magnetic field and zero temperature, regardless of the J_m for a dominant Heisenberg interaction ($J - J_2 < 0$).

Concluding the discussion of zero magnetic field properties in the case $J_m \neq 0$, we note, that when $J_m < 0$ (ferromagnetic coupling), the absolute value of J_m does not interfere with the ground state properties of the system (it will be two-fold degenerate ψ_{12} and ψ_{13} , if $J > J_2$ or ψ_5 and ψ_8 , if $J < J_2$).

Here then, we will discuss the regime $J - J_2 > 0$ introducing effects of the magnetic field H . We differentiate two subcases. First one, when $J_m \leq 2(J - J_2)$, one does not find magnetic entanglement in the system, since increasing the absolute value of

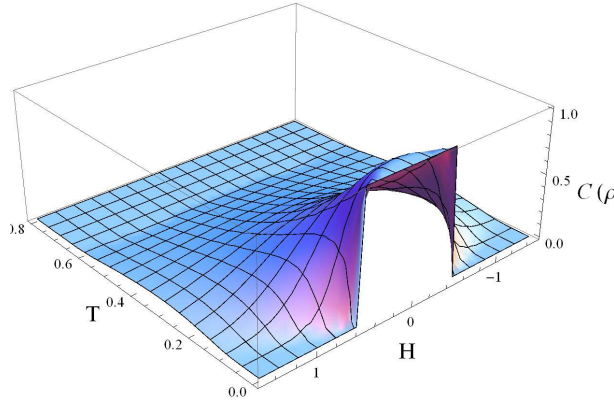


Figure 8. Concurrence $C(\rho)$ versus magnetic field H and temperature T for $J_2 = 1$ and $J = 1.5$ and $J_m = 1.5$.

magnetic field H , we obtain a sequence of separable states (e.g. $\psi_{12} \rightarrow (\psi_{10} + \psi_{11}) \rightarrow \psi_9$ or $\psi_{12} \rightarrow \psi_9$ for $H > 0$). Here and further by $(\psi_i + \psi_j)$ we will mean two-fold degenerate states.

Meanwhile, when $J_m > 2(J - J_2)$, the aforementioned sequence of states starts from $(\psi_6 + \psi_7)$ with maximum value of $C(\rho) = 1$, therefore we obtain magnetic entanglement (Fig. 8). One can introduce here critical values of magnetic field H_c^+ and H_c^- , corresponding to vanishing of magnetic entanglement. In contrary with the case $J_m = 0$, H_c^\pm does not coincide with the saturation fields H_s^\pm (see Sec. 2.1).

On the one hand, we have the ground state transitions $(\psi_6 + \psi_7) \rightarrow \psi_{12} \rightarrow (\psi_{10} + \psi_{11}) \rightarrow \psi_9$ (for $H > 0$) if the value of magnetic field, corresponding to the intersection of energies E_6 and E_{12} is lower than that of E_{10} and E_{12} [Fig. 9 (a)]. This condition gives: $J_m < 2J - J_2$. Thus the corresponding critical values of magnetic field can be found from $E_6 = E_{12}$ with $H_c^+ = 2J_2 - 2J + J_m$ (obviously, $H_c^- = -H_c^+$, from equation $E_6 = E_{13}$). On the other hand, when $J_m > 2J - J_2$, we have the ground state transitions $(\psi_6 + \psi_7) \rightarrow (\psi_{10} + \psi_{11}) \rightarrow \psi_9$ [Fig. 9 (b)]. Corresponding $H_c^+ = J_2$, found from $E_6 = E_{10}$ ($H_c^- = -J_2$, from $E_6 = E_{14}$). The ground state transition $(\psi_6 + \psi_7) \rightarrow \psi_9$ can not occur, since the corresponding condition is inconsistent with $J_m > 2J - J_2$.

Following the same technique as in previous paragraph (we will not stop on detailed phase structure), we obtain the following regimes for $J - J_2 < 0$: $H_c^+ = H_s^+ = J + J_2$ ($H_c^- = -H_c^+$) in the case $J_m < J_2 - J$ and $H_c^+ = 2J_2 - J_m$ if $J_2 > J_m > J_2 - J$, and finally, when $J_m > J_2$ one finds $H_c^+ = J_2$.

The special (boundary) case $J - J_2 = 0$ is also of interest, since one can observe here magnetic entanglement of different values ($C(\rho) = 1$ and $C(\rho) = 1/2$) (Fig. 10), whereas in the case $J_m = 0$, these two regimes cannot coexist for a fixed values of J and J_2 . This situation arises only for $0 < J_m < J$, when one finds the sequence of states $(\psi_6 + \psi_7) \rightarrow (\psi_5 + \psi_{12}) \rightarrow$ (factorable state) (for $H > 0$). In other words, at the values of magnetic field $H = \pm J_m$ (found from conditions $E_6 = E_{12}$ for $H > 0$ and $E_6 = E_8$ for $H < 0$) the states with different values of magnetic entanglement coexist.

As for the sudden-death temperature corresponding to the disappearing or arising of entanglement at non-zero magnetic field, one finds a similar behavior as in the case

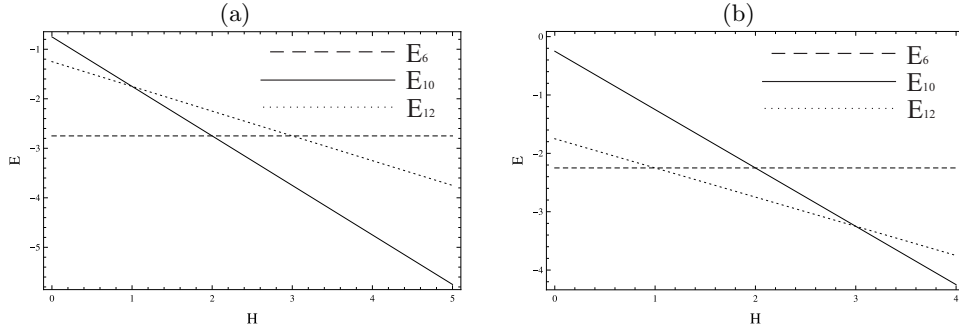


Figure 9. Eigenvalues E_6 , E_{10} and E_{12} versus magnetic field H for (a) $J_m < 2J - J_2$; (b) $J_m < 2J - J_2$.

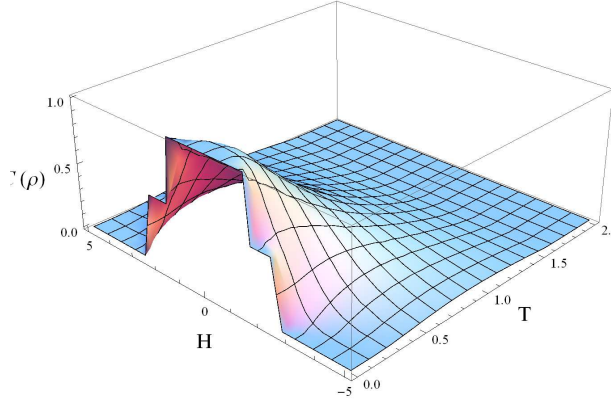


Figure 10. Concurrence $C(\rho)$ versus magnetic field H and temperature T for $J_2 = 2$ and $J = 2$ and $J_m = 1.5$.

$J_m = 0$, i.e. here again we find up to three sudden-death temperatures (as in Fig. 4), with a two peak behavior on the dependency of $C(\rho)$ on temperature.

4. Conclusion

In this paper we have studied the thermal entanglement of a spin-1/2 Ising-Heisenberg model on a symmetrical diamond chain, which has been proposed to understand a frustrated magnetism of the series of compounds, like $A_3Cu_3(PO_4)_4$ with $A=Ca, Sr, Bi_4Cu_3V_2O_{14}, Cu_3(TeO_3)_2Br_2$ and $Cu_3(CO_3)_2(OH)_2$. We have studied the phase structure and entanglement properties of the system in a wide range of Ising-type interaction constants $J_1 = J_3 \equiv J$, J_m and Heisenberg-type J_2 , considering that diamond chain structure describes a broad class of materials (within different values of exchange interaction parameters) and that the exact value of coupling constants for azurite ($Cu_3(CO_3)_2(OH)_2$) is still under scrutinizing question. Taking into account the classical and hence separable character of Ising-type interactions which are coupling adjacent Heisenberg dimers, we have calculated the entanglement of each of these

dimers separately. We have used the concurrence for quantifying the amount of entanglement between two Heisenberg-type spins, by tracing out Ising-type ones from the density matrix of the diamond-shaped cluster (the only entangled pair here is the Heisenberg dimer). The incorporation of next-nearest neighbor interaction J_m has also been investigated (generalized diamond chain) and the effects of external magnetic field have been invoked.

We have revealed a number of regimes with distinct ground state structure and qualitatively different thermodynamic behavior, depending on the relations between J, J_2 and J_m and values of magnetic field H . We found that in general for a dominant Heisenberg-type interaction ($J_2 > J$) the system's ground state is maximally entangled, but increasing the temperature, pure quantum correlations eventually disappears. On the other hand, for a dominant Ising-type interaction ($J > J_2$) the ground-state is non-entangled, whether the temperature gives rise to thermal entanglement. In the latter case one does not find magnetic entanglement at the absolute zero temperature (the system behaves as a classical one). However, magnetic field can lead to another, yet not described effect of two-peak behavior of concurrence $C(\rho)$ versus *temperature* with three sudden-death temperatures (one of them corresponding to reappearance of concurrence and the other two to its disappearing). These two peaks are separated by an area of a zero entanglement, which becomes narrower, with the growth of the magnetic field and aforementioned peaks merge into each other. Another novel effect was indicated for a boundary case $J = J_2$ when $0 < J_m < J$. Specifically, two states with different values of magnetic entanglement coexist for the value of magnetic field $H = \pm J_m$. One finds a step like behavior of concurrence versus magnetic field H , with plateaus at the value 1/2 and 1. In other words, the presence of competing interactions in the system and geometrical structure of the chain, each leading to a frustration, makes the phase structure of the system richer and gives rise to an interesting physical behavior. Finally, the adopted model guaranties an experimental realization for suitable theoretical treatment. Our results will be useful for further experimental detection of entanglement in the diamond chain structured macroscopic samples by means of entanglement witnesses (e.g. built from measurements of magnetic susceptibility [43]).

5. Acknowledgments

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